GROMACS - Bug #970

segfault in tip4pflex test case

07/13/2012 09:58 PM - Christoph Junghans

Status: Closed
Priority: High
Assignee: Berk Hess
Category: mdrun
Target version: 4.6
Affected version:
Affected version -
extra info:
512f97d29cb6e57851a4b7f037068c355
e8b72
Difficulty: uncategorized

Description

This happens in 50% of the cases for the tip4p{,flex} examples on my x86 laptop (Intel Core 2 Duo, T7100, gcc with gcc (Gentoo 4.6.3 p1.0, pie-0.5.1) 4.6.3).

Program received signal SIGSEGV, Segmentation fault.
sse_mask_init (order=4, work=0xb5313ce8) at
/home/christoph/votca/src/gromacs/src/mdlib/pme.c:2881
2881 work->mask_SSE0[of] = _mm_loadu_ps(tmp);
(gdb) bt
#0 sse_mask_init (order=4, work=0xb5313ce8) at
/home/christoph/votca/src/gromacs/src/mdlib/pme.c:2881
#1 gmx_pme_init (pmedata=0xb530676c, cr=0xb5303ab8, nnodes_major=1, nnodes_minor=2, ir=0x807e9b8, homenr=3072, bFreeEnergy=0, bReproducible=0, nthread=1) at /home/christoph/votca/src/gromacs/src/mdlib/pme.c:3164
#2 0x08054732 in mdrunner (nthreads_requested=0, fplog=0x807e378, cr=0xb5303ab8, nfile=36, fnm=0xbfffe1a8, oenv=0x807e2d8, bVerbose=0, bCompact=1, nstglobalcomm=1, ddyxz=0xbfffe7e4, dd_node_order=1, rdd=0, rconstr=0, dddlb_opt=0x807238d "auto", db_scale=0.800000012, ddcx=0x0, ddcy=0x0, ddcz=0x0, nstepout=100, resetstep=-1, nmultisim=0, repl_ex_nst=0, repl_ex_nex=0, repl_ex_seed=0, pforce=-1, ctp_period=15, max_hours=-1, deviceOptions=0x80704ba "", Flags=7168) at /home/christoph/votca/src/gromacs/src/kernel/runner.c:841
#3 0x0804e53f in main (argc=1, argv=0xbfffe9f4) at /home/christoph/votca/src/gromacs/src/kernel/mdrun.c:685

Roland's 1st clue was that the segfault on SSE intrinsic mean that the data isn't aligned sufficiently, so:
(gdb) print &tmp
$1 = (float (*)[8]) 0xbfffcb50
but it not the case.

Associated revisions

Revision 3ee63ecf - 07/17/2012 06:50 PM - Berk Hess
fix a segfault in sse_mask_init

- work array was unaligned in some cases
- fixes #970

Change-Id: I1b474019bf93e6ef6f7cc935aa3f732597a91a8

Revision 3ee63ecf - 07/17/2012 06:50 PM - Berk Hess
fix a segfault in sse_mask_init

- work array was unaligned in some cases
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History

#1 - 07/16/2012 05:37 PM - Berk Hess
What are the tip4p{,flex} examples exactly?
Have you run valgrind on this?

#2 - 07/16/2012 05:43 PM - Berk Hess
I think this is an alignment issue.
tmp doesn't need to be aligned, we are using loadu.
But mask_SSE0 should be aligned and I think putting an SSE register in a struct does not guarantee this.

#3 - 07/16/2012 05:55 PM - Berk Hess
- File pme.c added

Please try the patched version of pme.c attached.

#4 - 07/16/2012 05:56 PM - Christoph Junghans
Berk Hess wrote:

What are the tip4p{,flex} examples exactly?

These are two "complex" tests for the regressiontests repository.

Have you run valgrind on this?

No, just gdb, but if you tell me, what exactly you need I can provide it.

#5 - 07/16/2012 05:58 PM - Christoph Junghans
Berk Hess wrote:

Please try the patched version of pme.c attached.

It happens on my machine at home, I will test and come back.

#6 - 07/26/2012 01:31 AM - Roland Schulz
- Status changed from New to Closed

Files

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>pme.c</td>
<td>130 KB</td>
<td>07/16/2012</td>
<td>Berk Hess</td>
</tr>
</tbody>
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